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Preparing for the future of computing: bridging meso- and continuum within the ecascale materials codesign center

Belak, Jim, belak1@llnl.gov, Lawrence Livermore National Laboratory

ABSTRACT

The advent of Advanced/Additive Manufacturing and the Materials Genome Initiative has placed significant emphasis on accelerating the qualification of new materials for use in real applications. Within these workflows lies both the engineering scale qualification through building and testing components at scale and full-scale modeling with integrated continuum computer codes and the materials scale qualification through revolutionary methods to nondestructively measure microstructure (3DXRD) and physics specific experiments coupled with mesoscale mechanics simulations of the same physics specific experiment using the same microstructure. This is one of the use cases that drives the Exascale Materials Codesign Center (ExMatEx). The goal of the Codesign Center is very analogous to the acceleration of new materials deployment within the MGI, rather codesign accelerates the deploying of laboratory concepts for future computer components to enable a productive exascale computer system. To enable better mesoscale understanding in the continuum models, ExMatEx is creating a direct coupling between the continuum integrated code and direct numerical simulation of the mesoscale phenomena. Here, we review the ExMatEx project, its use cases and, in particular, the continuum <–> meso-scale coupling.

*PIs: Jim Belak and Tim Germann

http://science.energy.gov/ascr/research/scidac/co-design/

http://www.exmatex.org

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